

1,4-Naphthoquinone
130-15-4 | DTXSID5040704

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 58.7 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.42e-01

Confidence level: 6.41e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Hydroxymethylnaphthalene</div> <div>Measured: 148</div> <div>Predicted: 406</div>	<div>Image not found</div> <div>3,5-Dinitrobenzoic acid</div> <div>Measured: 33.9</div> <div>Predicted: 70.8</div>	<div>Image not found</div> <div>Phthalic anhydride</div> <div>Measured: 36.3</div> <div>Predicted: 38.0</div>
<div>Image not found</div> <div>Acetamide, N-(3-nitrophenyl)-</div> <div>Measured: 87.1</div> <div>Predicted: 89.4</div>	<div>Image not found</div> <div>2,2'-Dipyridyl</div> <div>Measured: 39.8</div> <div>Predicted: 56.3</div>	